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Fermi Surface Instability in Pr-based Skutterudites

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Skutterudite compounds have recently attracted much attention for improved thermoelectric materials and for the variety of the electrical and magnetic properties. $PrRu_4P_{12}$ shows a metal-insulator transition at $T_{\rm MI} = 60{\rm K}$. $PrFe_4P_{12}$ undergoes a non-magnetic ordering at $T_{\rm N} = 6.5{\rm K}$, then very heavy cyclotron masse larger than 60 m_0 have been found. The study for Fermi surface of $LaFe_4P_{12}$ indicates that the nesting with $q = (1, 0, 0)$ is likely in the compounds.* Very recently, structural phase transitions with $q = (1, 0, 0)$ are observed below $T_{\rm MI}$ or $T_{\rm N}$ in both of the above compounds.† Here the Fermi surfaces are calculated for Pr-based skutterudites, by using FLAPW and LDA+U method with assuming the singlet ground state in Pr^{3+}. The result is consistent with the physical properties in $PrFe_4P_{12}$, $PrRu_4P_{12}$ and $PrRu_4Sb_{12}$.

*H. Sugawara *et al.*: J. Phys. Soc. Jpn. **69** (2000) 2938.

†C.H. Lee *et al.*: J. Phys.: Condens. Matter **13** (2001) L45, K. Iwasa: private communications.